

Travaux

Bilan : 46 articles, 35 communications orales, 12 communications par affiche

Publications

Researcher ID : B-1525-2012 ; h-index : 13 au 15/02/15

Le « corresponding author » est indiqué par une étoile. Pour les publications postérieures à 2010, les facteurs d'impact (IF) de 2012 sont fournis.

P1. A. Pénicaud*, O. Y. Carreon, **A. Perrier**, D. J. Watkin, C. Coulon, “Supramolecular fullerene chemistry : synthesis, crystal structure and potassium intercalation of $[(C_{60})][C_6H_5)_2]$ ”, **J. Mater. Chem.**, 12 (2002), 913

P2. **A. Perrier**, D. Gourier, L. Joubert, C. Adamo*, “Spin trapping by bis(benzene)chromium: a density functional theory study”, **Phys. Chem. Chem. Phys.**, 5 (2003), 1337.

P3. **A. Perrier***, L. Bonnet, D. A. Liotard, J.-C. Rayez, “On the dynamics of H_2 desorbing from a Pt(111) surface “, **Surf. Sci.**, 581 (2005), 189.

P4. **A. Perrier***, L. Bonnet, J.-C. Rayez, “Dynamical study of H_2 and D_2 desorbing from a Cu(111) surface”, **J. Phys. Chem. A**, 110 (2006), 1608.

P5. **A. Perrier**, L. Bonnet*, J.-C. Rayez, “A Statistico-Dynamical Approach of rotational state distribution in associative desorptions “, **J. Chem. Phys.**, 124 (2006), 194701.

P6. C. Díaz*, **A. Perrier**, G.J. Kroes, “Associative desorption of N_2 from Ru(0001):A computational study”, **Chem. Phys. Lett.**, 434 (2007), 231.

P7. **A. Perrier***, F. Maurel, J. Aubard, “Theoretical investigation of the substituent effect on the electronic and optical properties of photochromic dithienylethene derivatives”, **J. Photochem. Photobiol. A**, 189 (2007), 167-176

P8. **A. Perrier***, F. Maurel, J. Aubard, “Theoretical study of the electronic and optical properties of photochromic dithienylethene derivatives connected to small gold clusters.”, **J. Phys. Chem A**, 111 (2007), 9688-98.

P9. F. Maurel, **A. Perrier**, E. A. Perpete, D. Jacquemin*, “A Theoretical Study of the Perfluoro-Diarylethenes Electronic Spectra.”, **J. Photochem. Photobiol. A** 199 (2008) 211-223

P10. **A. Perrier***, F. Maurel, E. A. Perpete, V. Wathélet, D. Jacquemin*, “Spectral Properties of Spirooxazine Photochroms: TD-DFT Insights”, **J. Phys. Chem. A**. 113 (2009) 13004–13012

P11. **A. Perrier***, L. Bonnet, J.-C. Rayez , “Transition state theory: a reaction dynamics tool applied to gas-surface reactions”, **L'Actualité Chimique** , 332 (2009) 27-35

P12. D. Jacquemin*, E. A. Perpète, F. Maurel and **A. Perrier***, “Ab Initio Investigation of the Electronic Properties of Coupled Dithienylethenes”, **J. Phys. Chem. Lett.** 1 (2010) 434-438 (IF = 6.59)

- P13.** D. Jacquemin*, E. A. Perpète, F. Maurel, **A. Perrier***, “*Doubly Closing or not? Theoretical Analysis for Coupled Photochromes*”, **J. Phys. Chem. C** 114 (2010) 9489-9497 (IF = 4.81)
- P14.** D. Jacquemin*, E. A. Perpète, F. Maurel and **A. Perrier***, “*Simulation of the Properties of a Photochromic Triad*”, **J. Phys. Chem. Lett.** 1 (2010) 2104-2108 (IF = 6.59)
- P15.** D. Jacquemin*, E. A. Perpète, F. Maurel, **A. Perrier**, “*TD-DFT Simulations of the Electronic Properties of Star-Shaped Photochromes*”, **Phys. Chem. Chem. Phys.** 12 (2010) 7994-8000 (IF = 3.83)
- P16.** D. Jacquemin*, C. Michaux, E. A. Perpète, F. Maurel, **A. Perrier**, “*Photochromic Molecular Wires: Insights from Theory*”, **Chem. Phys. Lett.** 488 (2010) 193-197
- P17.** S. Aloïse*, M. Sliwa, Z. Pawlowska, J. Réhault, J. Dubois, O. Poizat, G. Buntinx, **A. Perrier***, F. Maurel, S. Yamaguchi, M. Takeshita, “*Bridged Photochromic Diarylethenes Investigated by Ultrafast Absorption Spectroscopy: Evidence for Two Distinct Photocyclization Pathways*”, **J. Am. Chem. Soc.**, 132 (2010), 7379 – 7390 (IF = 10.68)
- P18.** D. Jacquemin*, E.A. Perpète, F. Maurel, **A. Perrier**, “*Hybrid Dithienylethene-Naphthopyran Multi-Addressable Photochromes: an Ab Initio Analysis*”, **Phys. Chem. Chem. Phys.** 12 (2010) 13144-13152 (IF = 3.83)
- P19.** F. Maurel, **A. Perrier**, D. Jacquemin*, “*An ab initio Simulation of a Dithienylethene/Phenoxynaphthacenequinone Photochromic Hybrid*”, **Journal of Photochemistry and Photobiology A: Chemistry** 218 (2011) 33-40 (IF = 2.42)
- P20.** **A. Perrier**, F. Maurel, I. Ciofini, D. Jacquemin* , “*A theoretical spectroscopy investigation of bifunctional platinum-bridged diarylethenes*”, **Chem. Phys. Lett.** 502 (2011) 77-81 (IF = 2.15)
- P21.** **A. Perrier***, F. Maurel, D. Jacquemin*, “*Interplay Between Electronic and Steric Effects in Multiphotochromic Diarylethenes*”, **J. Phys. Chem. C**, 115 (2011) 9193-9203 (IF = 4.81)
- P22.** Z. Pawlowska, A. Lietard, S. Aloïse*, M. Sliwa, A. Idrissi, O. Poizat, G. Buntinx, S. Delbaere, **A. Perrier**, F. Maurel, P. Jacques, J. Abe, “*The excited state dipole moments of betaine pyridinium investigated by an innovative solvatochromic analysis and TDDFT calculations*”, **Phys. Chem. Chem. Phys.** 13 (2011) 13185-13195 (IF = 3.83)
- P23.** **A. Perrier***, F. Maurel, D. Jacquemin*, “*Diarylethene–dihydroazulene multimode photochrome: a theoretical spectroscopic investigation*”, **Phys. Chem. Chem. Phys.** 13 (2011) 13791-13799 (IF = 3.83)
- P24.** **A. Perrier***, S. Aloïse*, Z. Pawlowska, M. Sliwa, F. Maurel, J. Abe, “*Photoinduced Intramolecular Charge Transfer Process of Betaine Pyridinium: a theoretical spectroscopic study*”, **Chem. Phys. Lett.**, 515 (2011) 42-48 (IF = 2.15)
- P25.** M. Cipolloni, A. Heynderickx, F. Maurel, **A. Perrier**, D. Jacquemin*, O. Siri, F. Ortica, G. Favaro*, “*A Multiswitchable Acidichromic and Photochromic Bisdiarylethene. An*

Experimental and Theoretical Study”, **J. Phys. Chem. C**, 115 (2011) 23096–23106 (IF = 4.81)

P26. D. Jacquemin*, E. A. Perpète, F. Maurel, **A. Perrier***, “*Photochromic properties of a dithienylethene–indolinoxazolidine switch: A theoretical investigation*”, **Computational and Theoretical Chemistry**, 963 (2011) 63-70 (IF = 1.37)

P27. **A. Perrier**, F. Maurel and D. Jacquemin* , “*Nature of the Excited-States in Large Photochromic Dimers: a TD-DFT Examination*”, **Chem. Phys. Lett.** 509 (2011) 129-133 (IF = 2.15)

P28. F. Maurel, **A. Perrier**, D. Jacquemin*, “*Ab Initio Modelling of Optical Spectra in pH-Sensitive Diarylethenes*”, **Int. J. Quantum Chem.** 112 (2012) 1122-1133 (IF = 1.37)

P29. S. Aloïse*, Z. Pawlowska, C. Ruckebusch, M. Sliwa, J. Dubois, O. Poizat, G. Buntinx, **A. Perrier**, F. Maurel, P. Jacques, J.-P. Malval, L. Poisson, G. Piani, J. Abe “*A two-step ICT process for solvatochromic betaine pyridinium revealed by ultrafast spectroscopy, multivariate curve resolution and TDDFT calculations*” **Phys. Chem. Chem. Phys.** 14 (2012) 1945-56 (IF = 3.83)

P30. R. Yasukuni*, R. Boubekri, J. Grand*, N. Félidj, F. Maurel, **A. Perrier**, R. Métivier, K. Nakatani, P. Yu, J. Aubard, “*Specific and Nondestructive Detection of Different Diarylethene Isomers by NIR-SERS*”, **J. Phys. Chem. C** 116 (2012) 16063–16069 (IF = 4.81)

P31. **A. Perrier***, S. Tesson, D. Jacquemin, F. Maurel, “*On the photochromic properties of dithienylethenes grafted on gold clusters*”, **Computational and theoretical chemistry**, 990 (2012) 167-176 (IF = 1.37)

P32. A. Fihey*, **A. Perrier**, F. Maurel, “*Tuning the optical properties of dithienylethenes: Theoretical insights*”, **J. Photochem. Photobiol. A**, 247 (2012) 30-41 (IF = 2.42)

P33. **A. Perrier**, F. Maurel, D. Jacquemin*, “*Single Molecule Multi-Photochromism with Diarylethenes*”, **Accounts of Chemical Research**, 45 (2012) 1173-1182 (IF = 20.83)

P34. G. Charron*, D. Hühn, **A. Perrier**, L. Cordier, C. J. Pickett, T. Nann, W. J. Parak, “*On the Use of pH Titration to Quantitatively Characterize Colloidal Nanoparticles*”, **Langmuir** 28 (2012) 15141-15149 (IF = 4.19)

P35. R. Boubekri, R. Yasukuni, S. Lau Truong, J. Grand, **A. Perrier**, J. Aubard, F. Maurel*, “*Raman study of a photochromic diarylethene molecule: a combined theoretical and experimental study*”, **Journal of Raman Spectroscopy**, 44 (2013) 1777–1785 (IF = 2.67)

P36. **A. Perrier**, F. Maurel, W. R. Browne, D. Jacquemin*, “*Full ring closing in a diarylethene hexamer: insights from theory*”, **Chem. Commun.**, 49 (2013), 4247-4249 (IF = 6.38)

P37. S. Aloïse*, M. Sliwa, G. Buntinx, S. Delbaere, **A. Perrier**, F. Maurel, D. Jacquemin, M. Takeshita, “*Do inverse DTEs behave as normal ones? A joint spectroscopic and theoretical investigation*”, **Phys. Chem. Chem. Phys.** 15 (2013), 6226-6234 (IF = 3.83)

P38. **A. Perrier***, S. Aloïse, M. Olivucci, D. Jacquemin, “*Inverse versus Normal Dithienylethenes : Computational Investigation of the Photocyclization Reaction*”, **J. Phys.**

Chem. Lett., 4 (2013) 2190-2196 (IF = 6.59)

P39. S. Aloïse*, Z. Pawlowska, O. Poizat, G. Buntinx, **A. Perrier**, F. Maurel, K. Ohkawa, A. Kimoto, J. Abe, “*Excited-state dynamics of thiophene substituted betaine pyridinium compounds*”, **Phys. Chem. Chem. Phys.** 16 (2014), 1460-1468 (IF = 3.83)

P40. A. Fihey*, F. Maurel, **A. Perrier***, “*Modeling the Absorbance Properties of a Pyrene Chromophore Grafted onto a Au₂₅ Nanocluster: A TD-DFT Study*”, **J. Phys. Chem. C** 118 (2014) 4444-4453 (IF = 4.81)

P41. A. Chantzis, J.Cerezo, **A. Perrier**, F. Santoro, and D. Jacquemin*, “*Optical Properties of Diarylethenes with TD-DFT: 0–0 Energies, Fluorescence, Stokes Shifts, and Vibronic Shapes*”, **J. Chem. Theory Comput.**, 10 (2014) 3944–3957 (IF = 5.31)

P42. A. Fihey*, B. Kloss, **A. Perrier*** and François Maurel, “*Density Functional Theory Study of the Conformation and Optical Properties of Hybrid Au_n-Dithienylethene Systems (n = 3, 19, 25)*”, **J. Phys. Chem. A**, 118 (2014) 4695–4706 (IF = 2.77)

P43. D. Mendive-Tapia*, **A. Perrier**, M. J. Bearpark, M. A. Robb, B. Lasorne, D Jacquemin , “*New insights into the by-product fatigue mechanism of the photo- induced ring-opening in diarylethenes*”, **Phys. Chem. Chem. Phys.**, 16 (2014) 18463-18471 (IF = 3.83)

P44. .A. Lietard, G. Piani, L. Poisson*, B. Soep, J.-M. Mestdagh, S. Aloïse, **A. Perrier**, D. Jacquemin, M. Takeshita, « *Competition direct vs indirect photochromism dynamics in constrained inverse dithienylethene molecules* », **Phys. Chem. Chem. Phys.** 16 (2014) 22262-22272 (IF = 3.83)

P45. A. Fihey*, F. Maurel, **A. Perrier***, “*A DFT study of a new class of gold nanocluster-photochrome multi-functional switches*”, **Phys. Chem. Chem. Phys.** 16 (2014) , 26240-26251 (IF = 3.83)

P46. S. Aloïse,* R. Yibin, I. Hamdi, G. Buntinx, **A. Perrier,*** F. Maurel, D. Jacquemin*, M. Takeshita “*The photochemistry of inverse dithienylethene switches understood*” **Phys. Chem. Chem. Phys.** 16 (2014) , 26762-26768 (IF = 3.83)

Communications Orales

• **Conférences invitées dans les congrès**

“Understanding the photoactivity of molecular switches within complex systems: a simple approach”, **A. Perrier**, Chemical Reactivity 2014: from accurate theories to simple models, Bordeaux (France), 21-23 Janvier 2014.

• **Séminaires invités** (*Le nom de l'orateur est souligné*)

I1. “Dynamics of molecular associative desorption: a theoretical study”, **A. Perrier**, L. Bonnet, J.-C. Rayez, Seminar, Laboratoire de Chimie Théorique, Université Aix-Marseille I, Marseille (France), 11th April 2006

I2. “Reactivity of molecular photoswitches in complex environments: ab initio spectroscopic studies”, **A. Perrier**, Wuhan University, College of Chemistry, Wuhan (**China**), 3 juillet 2013.

- I3.** “Development of new methods to model the optical properties of nanometer-sized gold nanoparticle/photochrome hybrid systems”, A. Fihey, **A. Perrier**, F. Maurel, Bremen Computational Center for Material Science, Bremen (**Allemagne**), 28 Oct. 2013
- I4.** “Les photochromes couplés : un exemple d’application de la spectroscopie *ab initio* », A. Perrier, F. Maurel, E. Perpète , D. Jacquemin, Cachan (Fr.), 30 janvier 2012.
- I5.** “Modélisation de la réactivité et des propriétés optiques de molécules photochromes au sein de systèmes complexe », A. Perrier, A. Fihey, F. Maurel, D. Jacquemin, Chimie Paris Tech (Fr.), 27 novembre 2012,
- I6.** “ Modelling the optical properties of photochromic molecules within complex systems: The example of photochromes grafted onto gold nanoparticles», A. Perrier, Equipe Modes, Laboratoire CEISAM, Université de Nantes (Fr.), 7 mars 2013
- I7.** “Modélisation Moléculaire: de la théorie aux expériences”, A. Perrier, Summer School of the Master “Frontiers of Chemistry”, Fontainebleau (Fr.), 5 septembre 2013.
- I8.** “Photoactivity of molecular switches within complex systems: Insights from theory”, A. Perrier, Séminaires autour des Nanosciences – SCAN,UFR de Chimie, Université Paris Diderot, Paris (Fr.), 18 octobre 2013.

• **Communications** (*Le nom de l’orateur est souligné*)

- C1.** “Kinematic rotations in RRKM theory”, A. Perrier, L. Bonnet, J.-C. Rayez, 2nd European School on Computational Chemistry, Reaction and Molecular Dynamics, Barcelona (Spain), 23rd -28th June 2003
- C2.** “New perspective in Transition State Theory”, J.C. Rayez, **A. Perrier**, P. Larrégaray and L. Bonnet, 3rd International Meeting on Photodynamics , La Havana (Cuba), 16th-20th February 2004
- C3.** “Dynamics of molecular associative desorption”, A. Perrier, L. Bonnet, J.-C. Rayez, 7^{èmes} Journées Francophones des Jeunes Physico-Chimistes, Monastir (Tunisia), 19th-21st March 2004
- C4.** “Statistico-Dynamical Approach of Chemical Reaction Dynamics”, L. Bonnet, P. Larregaray, **A. Perrier**, J.C. Rayez , Stereodynamics 2004 - Stereodynamics of Chemical reactions, Osaka (Japan), 28th November -3rd December 2004
- C5.** “On the dynamics of molecular associative desorption “, A. Perrier, L. Bonnet, J.-C. Rayez, Graduate Research Seminar on Molecular Energy Transfer, Gordon Research Conference, Buellton (California, USA), 9th January 2005
- C6.** « New perspective in Transition State Theory », J.C. Rayez, P. Larrégaray, L. Bonnet, **A. Perrier**, 7th WATOC 2005 Congress, Captown (South Africa), 16th – 21st January 2005
- C7.** “The statistico-dynamical approach : a transition state theory revisited “, J. C. Rayez, L. Bonnet, P. Larrégaray, **A. Perrier**, Workshop in Honor of Antoine Salin : Recents Advances on the Dynamics of Atomic and Molecular Particles interacting with Gas and Solid Targets, San Sebastien Donostia (Spain) 24th- 26th October 2005
- C8.** “The Statistico - Dynamical Approach :a Transition state Theory revisited. Application to

molecular associative desorptions”, J. C. Rayez, L. Bonnet, P. Larrégaray, **A. Perrier**, 4th Congress on Photodynamics - La Havana (Cuba) 31st January – 13th February 2006

C9. “Optical properties of photochromic molecules connected to gold clusters: towards hybrid nano-switches”, **A. Perrier**, F. Maurel, J. Aubard, X^{èmes} Rencontres des Chimistes Théoriciens Francophones, Nancy (France), 10th -13th July 2006

C10. “La réactivité chimique du point de vue de la Théorie de l’Etat de Transition”, L. Bonnet, P. Larrégaray, **A. Perrier** et J.C. Rayez, X^{èmes} Rencontres des Chimistes Théoriciens Francophones, Nancy (France), 10th -13th July 2006

C11. “La théorie de l’état de transition et la réactivité chimique / Transition State Theory and Chemical Reactivity”, J. C. Rayez, L. Bonnet, P. Larrégaray et **A. Perrier**, 32^{ème} CHITEL – Cartagena (Tunisia), 1st - 6th September 2006

C12. “Theoretical study on optical properties of photochromic molecules functionalized by gold nanoparticles : towards molecular plasmonic devices”, **A. Perrier**, F. Maurel, J. Aubard, Japan-France Joint Seminar on Photochromism: Switches and Memories, Honan Village, 15th-18th October 2006

C13. “Quantum Modeling of a Dithienylethene Biomimetic Photochemical Switch”, **A. PERRIER**, C. RAYNAUD, A. SINICROPI, N. FERRE, M. OLIVUCCI, 2007 International Symposium on Photochromism (ISOP-07), Vancouver (Canada), October 7-10 2007.

C14. “Approche statistique de la dynamique réactionnelle : des processus triatomiques aux réactions élémentaires gaz-surface », P. LARREGARAY, L. BONNET, **A. PERRIER**, J.C. RAYEZ , 11ème Rencontre des Chimistes Theoriciens Francophones (RCTF-2009), Dinard, France, 30 june – 4 july 2008

C15. “Développement de dispositifs plasmoniques moléculaires photo-modulables », BOUBEKRI R., **PERRIER A.**, GRAND J., AUBARD J. MAUREL F., 10èmes Journées Francophones des Jeunes Physico-Chimistes, Ambleteuse, France, 18-22 october 2009

C16. «Development of photo-driven molecular plasmonic devices», BOUBEKRI R., BROSSEAU A., **PERRIER A.**, GRAND J., AUBARD J. MAUREL F., International workshop on organic Photoswitchable Multifunctional molecules and materials, Shangai, China, 25-27 october 2009.

C17. “Bridged Photochromic diarylethenes investigated by femtosecond spectroscopy:evidences for two distinct photocyclization pathways”, ALOISE S., SLIWA M., PAWLOWSKA Z., REHAULT J., POIZAT O., BUNTINX G., **PERRIER A.**, MAUREL F., TAKESCHITA M., Fisphoton 2009 – 2nde France-Italy Symposium on Photosciences, Marseille (France), 7-10 december 2009.

C18. “Etude théorique des propriétés électroniques des photochromes couplés : quand la fermeture se coince... », **A. PERRIER**, F. MAUREL, E. PERPETE, D. JACQUEMIN, 12ème Rencontre des Chimistes Theoriciens Francophones (RCTF-2010), Namur (Belgium), 4-8 july 2010

C19. “TD-DFT simulations of coupled photochroms”, **A. Perrier**, F. Maurel, D. Jacquemin, Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela (Spain), 16-22 july 2011

C20. “Fluorescence photoswitching at the nanoscale based on photochromism”, R. METIVIER, J. PIARD, **A. PERRIER**, J. SU, K. OUHENIA, S. MAISONNEUVE, A. JACQUART, J. XIE, P. YU, F. BRISSET, T. FUKAMINATO, K. NAKATANI, Central European Conference on Photochemistry CECP-2012, Bad Hofgastein (Austria), 5-9 february 2012

C21. “Ab initio models for multi-photochromic entities”, D. JACQUEMIN, **A. PERRIER**, F. MAUREL, CECAM Workshop "New QM/MM opportunities for in silico macromolecular photochemistry", Lyon (France), 28 february-2 march 2012

C22. “ Photochimie de betaine pyridinium solvatochromes étudiée par spectroscopies ultrarapides et calculs TDDFT.”, S. ALOISE, Z. PAWLOWSKA, C. RUCKEBUSCH, M. SLIWA, O. POIZAT, **A. PERRIER**, F. MAUREL, P. JACQUES, J. ABE, J.-P. MALVAL, Journées de printemps du Groupe Français de Photochimie, photophysique et photosciences, Bordeaux (France), 31 may-1st june 2012

C23. “ Can photochromic molecules anchored on gold nanoparticles act as nano-hybrid switches?”, A. PERRIER, S. TESSON, A. FIHEY, D. JACQUEMIN, F. MAUREL, Second edition of the International Conference on Advanced Materials Modelling (ICAMM), Nantes (France) 13-16 june 2012

C24. “Modification des propriétés optiques de composés photochromes : un exemple d'application de la spectroscopie *ab initio*.”, A. FIHEY, **A. PERRIER**, F. MAUREL, Journée thématique de l'Ecole Doctorale 388 consacrée à la “Spectroscopie: Méthodologie et Applications”, 28 june 2012, Paris (France).

C25. “Etude physico-chimique de la complexation du Fer par des sidérophores synthétiques”, N.-T. Ha-Duong, S. Abdelsayed, N. Serradji, M. Hémadi, J.-M. El Hage Chahine, V. Kosyova, G. Basuyaux, J. Hénault, C. Z. Dong, **A. Perrier**, P. Verbeke, 13èmes Journées Francophones des Jeunes Physico-Chimistes, Dinard (France), 15-19 october2012

C26. “Ultrafast Relaxation Dynamics of isolated photochromic molecules”, A. Lietard, S. Aloïse, **A. Perrier**, L. Poisson, J-M Mestdagh, B. Soep, M. Takeshita, Phenics International Network Symposium 2012, Nantes (France), 28 november -1st December 2012

C27. “Multiphotochromic devices: an *ab initio* spectroscopic study”, **A. Perrier**, F. Maurel, D. Jacquemin, Phenics International Network Symposium 2012, Nantes (France), 28 november -1st December 2012

C28. “Accéder à la photophysique d'un système hybride Nanoparticule/ Photochrome : un défi pour les calculs quantiques”, A. Fihey, **A. Perrier**, F. Maurel, Journée de l'Ecole Doctorale 388 « Chimie Physique et Chimie Analytique de Paris Centre », Paris (France), 25 april 2013

C29. “Etude théorique des propriétés optiques de composés hybrides photoactifs”, A. Fihey, **A. Perrier**, F. Maurel, Journées Modélisation 2013, Paris (France), 30 may 2013

C30. “Modeling the optical properties of nanometer-sized gold nanoparticle/photochrom hybrid systems: a challenge for quantum chemistry”, A. Fihey, **A. Perrier**, F. Maurel, International Symposium on Photochromism ISOP-Phenics 2013, Berlin (Germany), 23-26 septembre 2013

C31. “Modélisation des propriétés optiques de systèmes hybrides nanoparticule/photochrome de taille nanométrique : Un défi pour la chimie quantique.”, A. Fihey, **A. Perrier**, F. Maurel,

Groupe français de photochimie, photophysique et photosciences (GFP2P), Orsay (France), 12-13 novembre 2013.

C32. « Modélisation multi-échelle des propriétés optiques de systèmes hybrides nanoparticule/photochrome: de la TD-DFT au couplage Mécanique Quantique/Electrodynamique », A. Fihey, **A. Perrier**, F. Maurel, 14èmes Rencontres des Chimistes Théoriciens Francophones (RCTF 2014), Paris, 30 juin – 4 juillet 2014

C33. « Optical properties of diarylethenes with TD-DFT : 0-0 energies, fluorescence, stokes shifts and vibronic shapes », A. Chantzis, J. Cerezo, **A. Perrier**, F. Santoro, D. Jacquemin, XXVth IUPAC Symposium on Photochemistry, Bordeaux (France) 13-18 juillet 2014

C34. “The photochemistry of inverse dithienylethene switches understood”, S. Aloïse, R. Yibin, I. Hamdi, G. Buntinx, **A. Perrier**, F. Maurel, D. Jacquemin, M. Takeshita, 9th PHENICS International Network Symposium, Bordeaux (France) 18-19 juillet 2014

C35. “Modeling the optical properties of organic photoswitch / gold nanoparticle hybrid systems”, **A. Perrier**, A. Fihey, F. Maurel, I. Ciofini, C. Adamo, CODECS 2014; Advances in Computational Spectroscopy, Bratislava (Slovaquie), 23-27 octobre 2014

Communication par affiches

A1. “Spin trapping by bis(benzene)chromium: a density functional theory “, **A. Perrier**, D. Gourier, L. Joubert, C. Adamo , Fourth Congress of the International Society for Theoretical Chemical Physics, Marly-le-Roi (France), 9th-16th July 2002

A2. “A theoretical study of H₂ and D₂ desorbing from a Cu(111) surface “, **A. Perrier**, L. Bonnet, J.-C. Rayez, Donastia International Physics Center Workshop: Molecule-Surface Interactions: Elementary Reactive Processes, San Sebastian (Spain), 7th -11th September 2004

A3. “On the dynamics of molecular associative desorption”, **A. Perrier**, L. Bonnet, J.-C. Rayez, Gordon Research Conference on Molecular Energy Transfer, Buellton (California, USA), 9th -14th January 2005

A4. “Raman spectra of a photochromic diarylethene molecule: a combined theoretical and experimental study.” BOUBEKRI R. , SPANGENBERG A. BROSSEAU A., YU P. ,LAU-TRUONG S., GRAND J., **PERRIER A.**, AUBARD J., MAUREL F. JSPS and CNRS Seminar, New Horizons of Photochromism From Design of Molecules to Applications, Arras (France) , 12-15 october 2008

A5. “Theoretical study on optical properties of photochromic molecules functionalized by gold nanoparticules: towards nano-hybrid switches.”, **PERRIER A.**, BOUBEKRI R., MAUREL F., 13th edition of the International Conference on the Applications of Density Functional Theory in Chemistry and Physics, Lyon (France), 31 august - 4 september 2009

A6. “Optical Properties of Photochromic Molecules Functionalized by Gold Clusters”, **PERRIER A.**, BOUBEKRI R., MAUREL F., Ab initio Modelling in Solid State Chemistry (MSSC2010), London (UK), 13-17 september 2010

A7. “Photoinduced Intramolecular Charge Transfer Process of pyridinium betaine: a theoretical spectroscopic study”, **A. Perrier**, Z. Pawlawska, F. Maurel, S. Aloïse, Ninth

Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela (Spain), 16-22 July 2011

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